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**A THERMODYNAMIC SURFACE FOR
WATER: THE FORMULATION AND
COMPUTER PROGRAMS**

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NATIONAL BUREAU OF STANDARDS, Ernest Ambler, *Director*

A Thermodynamic Surface for Water: The Formulation and Computer Programs

by

Lester Haar, John S. Gallagher and George S. Kell

1. Introduction

This report has been prepared to provide computational details and computer programs for the evaluation of the thermodynamic properties of water and steam. It is based on an extensive correlation of thermodynamic properties.¹ Included herein are the basic equations for the description of the thermodynamic properties of water and detailed listings of computer programs based on these equations. With this information, thermodynamic properties can be calculated from the freezing point to 2500 K in temperature and from the dilute gas to well in excess of 1 GPa (10,000 bars) in pressure for liquid and gaseous states for undissociated water.

In reducing the data the molecular weight of ordinary water has been taken as 18.0152 g mol⁻¹,² the universal gas constant as 8.31441 J mol⁻¹ K⁻¹, and hence the specific gas constant as 0.461522 J g⁻¹ K⁻¹.³ Absolute temperatures on the International Practical Temperature Scale of 1968 have been used as the realization of the thermodynamic scale.

This report contains five sections and 2 appendices: A brief discussion of the structure of the thermodynamic surface for water is given in section 2, and in section 3 are the equations, parameters and constants that define the surface. Section 4 contains the thermodynamic relations used in the computer program. It also contains a discussion

of the general organization and structure of the computer program. Section 5 contains statements regarding the accuracy and range of validity of our surface. In Appendix A are the computer listings and a guide to their use, and, lastly, in appendix B, is a printout of calculations obtained with the program, so that the user can check his results.

2. Structure of the thermodynamic surface

The thermodynamic surface is composed of three parts: (1) The first, referred to as the base function, is obtained from a theoretical equation of state.⁴⁻¹² It properly describes the low-density vapor, the high temperature behavior at all densities, and the dense fluid at all temperatures. Except for a large region around the critical point, the base function yields results that are at least in semi-quantitative accord with data. (2) The second, referred to as the residual function, yields corrections to the base function. These corrections are small in regions where the base function is in good accord with data, and in regions beyond the range of the data. The contributions to the pressure from the base function and the residual function are readily integrable in closed form to yield their respective contributions to the Helmholtz function. (3) The third includes the thermodynamic properties for the ideal gas state. These have been reported recently by Woolley¹³ as part of a detailed analysis of the rotation-vibration structure of the water molecule.

A major part of the work was given to the derivation of the 40 terms that form the residual function. The first 36 terms were used in a global, least squares fit to data. Each of these terms yields important contributions over wide ranges of the independent variables. Following this, small improvements were made by adding 3 terms that contribute

only in the immediate neighborhood of the critical point, and a single term that contributes only in the region of high pressures and low temperatures. Except in these very limited regions, the residual function is given by the first 36 terms. A discussion of the thermodynamic surface obtained with the residual function so restricted (terms 1-36) is given in reference [12].

The three parts are combined to obtain the expression for the Helmholtz function for fluid water,

$$A(\rho, T) = A_{\text{base}}(\rho, T) + A_{\text{residual}}(\rho, T) + A_{\text{ideal gas}}(T), \quad (1)$$

where the independent variables are density (ρ) and temperature (T).

Eq. (1) is what we mean when we refer to the thermodynamic surface for water.

3. The Helmholtz function

Presented in this section are the equations that define the Helmholtz function Eq (1). The units used for the independent variables are ρ (g/cm³) and T (K), and R (J g⁻¹ K⁻¹) for the specific gas constant, so that $A(\rho, T)$ is given in joules/g.

The base function:

$$A_{\text{base}}(\rho, T) = RT \left\{ -\ln(1-y) - \frac{\beta-1}{1-y} + \frac{\alpha+\beta+1}{2(1-y)^2} + 4y \left(\frac{B}{b} - \gamma \right) - \frac{\alpha-\beta+3}{2} + \ln \frac{\rho RT}{P_0} \right\}, \quad (2)$$

where α , β , and γ are geometric constants 11, 133/3 and 7/2; y is a dimensionless density, given by $y = b\rho/4$, and $P_0 = .101325 \text{ MPa} \equiv 1 \text{ atmosphere}$.

The parameter b is a temperature dependent hard sphere volume, and B is related to the second virial coefficient,

$$b = b_1 \ln \frac{T}{T_0} + \sum_{0,3,5} b_i \left(\frac{T_0}{T} \right)^i, \quad (3)$$

$$B = \sum_{0,1,2,4} B_i \left(\frac{T_0}{T} \right)^i, \quad (4)$$

where $T_0 = 647.073$ K and the coefficients b_i and B_i are listed in table 1.

Table 1

$b_i (\text{cm}^3 \text{ g}^{-1})$	i	$B_i (\text{cm}^3 \text{ g}^{-1})$
.7478629	0	1.1278334
-.3540782	1	-.5944001
0	2	-5.010996
.007159876	3	0
0	4	.63684256
-.00352836	5	0

The residual function:

$$A_{\text{residual}}(\rho, T) = \sum_{i=1}^{36} \frac{g_i}{k(i)} \left(\frac{T_0}{T} \right)^{\ell(i)} (1 - e^{-a\rho})^{k(i)} + \sum_{i=37}^{40} g_i \delta_i^{\ell(i)} \exp \left[-\alpha_i \delta_i^{k(i)} - \beta_i \tau_i^2 \right], \quad (5)$$

where $a = 1 \text{ cm}^3/\text{g}$, and the g_i are coefficients determined by fits to data. The quantities δ_i and τ_i are reduced densities and temperatures, respectively, given by

$$\delta_i = \frac{\rho - \rho_i}{\rho_i}, \quad \tau_i = \frac{T - T_i}{T_i},$$

and ρ_i , T_i are specified density and temperature values. The $k(i)$ and $\ell(i)$ are integers. Values for the constants and parameters for the residual function are listed in table 2.

Table 2

i	k(i)	l(i)	g(i) (J g ⁻¹)	i	k(i)	l(i)	g(i) (J g ⁻¹)
1	1	1	-.530629685290+03	19	5	4	-.138025771779+07
2	1	2	.227449014244+04	20	5	6	-.251099143690+06
3	1	4	.787793330207+03	21	6	1	.465618261156+07
4	1	6	-.698305273750+02	22	6	2	-.727527732754+07
5	2	1	.178638328754+05	23	6	4	.417742461483+06
6	2	2	-.395147315633+05	24	6	6	.140163582446+07
7	2	4	.338038842808+05	25	7	1	-.315552313921+07
8	2	6	-.138550502027+05	26	7	2	.479296663846+07
9	3	1	-.256374366133+06	27	7	4	.409126647812+06
10	3	2	.482125759814+06	28	7	6	-.136263693884+07
11	3	4	-.341830169697+06	39	9	1	.696252208627+06
12	3	6	.122231564174+06	30	9	2	-.108349000964+07
13	4	1	.117974336558+07	31	9	4	-.227228274017+06
14	4	2	-.217348101104+07	32	9	6	.383654860007+06
15	4	4	.108299521686+07	33	3	0	.688332579443+04
16	4	6	-.254419980640+06	34	3	3	.217572455226+05
17	5	1	-.313777749478+07	35	1	3	-.266279448298+04
18	5	2	.529119107577+07	36	5	3	-.707304180821+05

i	k(i)	ℓ(i)	ρ _i (g/cm ⁻³)	T _i (K)	α _i	β _i	g _i (J g ⁻¹)
37	2	0	.319	640.	34	20000	-.225
38	2	2	.319	640.	40	20000	-1.68
39	2	0	.319	641.6	30	40000	.055
40	4	0	1.55	270.	1050	25	-93.0

The ideal gas function:

$$A_{\text{ideal gas}}(T) = -RT \left\{ 1 + \left(\frac{C_1}{T_R} + C_2 \right) \ln T_R + \sum_{i=3}^{18} C_i T_R^{i-6} \right\} \quad (6)$$

where $T_R = T/100$ K.

The coefficients C_i are given in table 3.

Table 3

i	C_i
1	.197302710180+02
2	.209662681977+02
3	-.483429455355+06
4	.605743189245+05
5	.225602388500+02
6	-.987532442000+01
7	-.431355385532-01
8	.458155781927-04
9	-.477549017624-07
10	.412384608402-10
11	-.279290527404-13
12	.144816952031-16
13	-.564736589529-20
14	.162004460052-23
15	-.330382277656-27
16	.451916066716-31
17	-.370734122641-35
18	.137546067535-39

The Eqs 1 thru 6 and the values for the coefficients and parameters included in this section contain the complete thermodynamic description for water. Since $A(\rho, T)$ is everywhere analytic, it is straightforward to evaluate appropriate derivatives and to obtain closed-form expressions

for all thermodynamic properties over the entire fluid range. In the next section is a discussion of how this is done.

4. Method of calculation and the computer program

The thermodynamic quantities are calculated from $A(\rho, T)$ using the following relations:

$$P = \rho RTZ = \rho^2 \frac{\partial A}{\partial \rho} \quad (\text{Pressure}) \quad (7)$$

$$\frac{\partial P}{\partial \rho} = \frac{2}{\rho} P + \rho^2 \frac{\partial^2 A}{\partial \rho^2} \quad (8)$$

$$\frac{\partial P}{\partial T} = \rho^2 \frac{\partial^2 A}{\partial \rho \partial T} \quad (9)$$

$$S = - \frac{\partial A}{\partial T} \quad (\text{entropy}) \quad (10)$$

$$U = A + TS \quad (\text{internal energy}) \quad (11)$$

$$H = U + P/\rho \quad (\text{enthalpy}) \quad (12)$$

$$C_V = - T \frac{\partial^2 A}{\partial T^2} \quad (\text{isochoric heat capacity}) \quad (13)$$

$$G = A + P/\rho \quad (\text{Gibbs functions}) \quad (18)$$

$$C_P = C_V + \frac{T}{\rho^2} \left(\frac{\partial P / \partial T}{\partial P / \partial \rho} \right)^2 \quad (\text{isobaric heat capacity}) \quad (19)$$

$$\omega = \left(C_P / C_V \frac{\partial P}{\partial \rho} \right)^{1/2} \quad (\text{speed of sound}) \quad (20)$$

$$B_{II} = \frac{1}{2RT} \left(\frac{\partial^2 P}{\partial \rho^2} \right)_{\rho=0} \quad (\text{2nd virial coef.}) \quad (21)$$

$$\frac{dB_{II}}{dT} \quad (22)$$

$$\delta_T \equiv \left(\frac{\partial H}{\partial P} \right)_T = \frac{1}{\rho} - \frac{T}{\rho^2} \frac{\partial P / \partial T}{\partial P / \partial \rho} \quad (\text{isothermal J-T coef.}) \quad (23)$$

$$\delta_H \equiv \left(\frac{\partial T}{\partial P} \right)_H = \frac{\delta_T}{C_P} \quad (\text{Joule-Thomson coef.}), \quad (24)$$

where except as indicated otherwise all dependent variables are functions of ρ and T . Since Eqs 7 thru 18 are linear in $A(\rho, T)$ each can be represented as the sum of contributions from its three parts.

The computer print-out in appendix A is the FORTRAN 77 program for calculating thermodynamic properties based on the equations contained in this report. All calculations related to the same part of $A(\rho, T)$ are included in the same sub-routine. Thus the sub-routine "BASE" includes Eqs (2-4) for the contribution from the base function to the Helmholtz function, plus each of the contributions therefrom to Eqs 7 thru 18. Similarly the sub-routine "QQ" includes all such contributions from the residual function, and sub-routine "IDEAL" contains the contributions from the ideal gas. Because the detailed equations are easily "read" from the respective sub-routines they are not reproduced here.

The contributions to the various thermodynamics properties Eqs 7-24 are summed in sub-routine "THERM". Also included are routines for properties associated with liquid-vapor coexistence. All calculations are referred to the liquid at the triple point, for which state the internal energy and entropy are zero. Though the units for the calculations are $\rho(\text{g/cm}^3)$, $T(\text{K})$ and joules, routine "UNIT" is included which allows use of other units. Lastly, the iteration sub-routine "DFIND" allows access with independent variables P and T .

All equations, including parameters and constants listed in sections 2 thru 4 are included in the program listing in Appendix A. Should any inconsistencies be found between the text and Appendix A, it is likely that the errors are in the text. Please let us know if you discover any.

5. Discussion

The data selected for the derivation of the thermodynamic surface were primarily P_oT data. These cover the range from $0^\circ \leq t \leq 1000^\circ\text{C}$ and $0 \leq P \leq 1000 \text{ MPa}$. Other kinds of data used include values for the enthalpy of the saturated liquid and for the isothermal compressibility of the liquid below 100°C . No mathematical constraints were used to impose exact accord with pre-assigned values. The surface yields values consistent with all input data within reasonable estimates of their tolerance. It has been further validated by extensive comparison with high quality thermodynamic data, including other than P_oT that had not been used in the derivation of the surface.

At very high pressure and at very high temperatures thermodynamic values calculated with the surface are in accord with those given by the (theoretical) base function, so that the surface should yield useful estimates well beyond the range of the data used in its derivation. Thus, except very close to the melting curve, the surface should remain quantitative at pressures equal to 2000 MPa and at least semi-quantitative to 4000 MPa, for temperatures in the range $250 \leq t \leq 2500 \text{ K}$ for undissociated fluid water. Lastly, because the surface is analytic, it yields some results at the critical point and its immediate neighborhood which are at variance with what modern theory predicts. Though we have not found significant departure from any reliable critical region data, we caution that the surface may not conform to all theoretical expectations in the region defined by

$$\begin{aligned} T &= T_c \pm 0.5 \text{ K} \\ \rho &= \rho_c (1 \pm .2) \end{aligned} \quad ,$$

where T_c and ρ_c are values at the critical point.

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APPENDIX A

This appendix contains the FORTRAN 77 programs which yield values for thermodynamic properties for liquid and gaseous states for water. The independent variables are temperature (T) and density (D). The programs should yield useful results in the range

$$250 \leq T(K) \leq 2500$$

$$10^{-8} \leq D(\text{g/cm}^3) \leq D(P_{\text{max}}),$$

where P_{max} is the lesser of the pressure of melting ice or 4000 MPa. For values of density less than or equal to 10^{-8} g/cm^3 , the program sets the density of 10^{-8} g/cm^3 .

Outlined below are the procedures for use of the subroutines which follow. In this outline, the symbol used for pressure is "P", for density is "D", and for temperature is "T". Calculations are made in the internal units of the program which are MPa, g/cm³ and deg K respectively. See III below for conversions to other units. Examples of the use of these routines are given in three main programs in Appendix B, with samples of the output which can be used for checking the implementation of the programs.

I. For Density and Temperature as independent variables, the sequence

```
CALL BB(T)
CALL BASE(D,T)
CALL QQ(T,D)
```

will place quantities in COMMON from which

$$P = D * GASCON * T * ZB + Q0$$

$$dP/dD = GASCON * T * (ZB + Y * DZB) + Q5$$

To obtain the other thermodynamic properties:

```
CALL THERM(D,T)
```

will place in COMMON "AD" (=A/RT), "GD" (=G/RT), "SD" (=S/R), "UD" (=U/RT), "HD" (=H/RT), "CVD" (=C_v/R), "CPD" (=C_p/R), "DPDT" (=dP/dT, MPa/K), "DVDT" (=dV/dT, cm³/gK), "CJTT" (isothermal joule-thompson coeff, cm³/g) and "CJTH" (adiabatic joule-thompson coeff, K/MPa). These properties in the desired units can then be obtained by R or RT as appropriate in the desired units.

II. Pressure and Temperature as independent variables

```
CALL DFIND(DOUT,P,DGUESS,T,DPDD)
```

This will return the density corresponding to the input P and T as DOUT from which the procedures in I can be used for further calculations. This routine requires an initial approximate guess for the density for use to begin the Newton iteration. dP/dD is also returned as a byproduct.

III. Use of other systems of units.

A group of three subroutines is included which facilitate the use of a system of units chosen by the user:

```
CALL UNIT
```

will query the user as to which units are desired for temperature, pressure, density and energy, and set up the necessary parameters for converting from the desired units to the internal units and back again for the output. The names of the units in alphanumeric characters are also placed in COMMON for use in labeling.

```
FUNCTION TTT(Texternal), and
```

```
FUNCTION TTI(Tinternal)
```

will convert from external T to deg K, and from deg K to the external T respectively.

BLOCK DATA

implicit double precision(a-h,o-z)

real p,q

COMMON /ACONST/ WM,GASCON,TZ,AA,ZP,DZB,YB,UREF,SREF

COMMON /NCONST/ G(40),II(40),JJ(40),NC

COMMON /ELLCN/ G1,G2,GF,B1,B2,B1T,B2T,B1TT,B2TT

COMMON /BCONST/ P(10),Q(10)

COMMON /ADDCN/ ATZ(4),ADZ(4),AAT(4),AAD(4)

C THIS BLOCKDATA SUBROUTINE SUPPLIES MOST OF THE FIXED PARAMETERS
 C USED IN THE REST OF THE ROUTINES. P IS THE b(1) of TABLE I,
 C Q IS THE B(1) OF TABLE I, G1,G2 AND GF ARE THE ALPHA, BETA
 C AND GAMMA OF EQ 2, AND G,II,JJ ARE THE g(1), k(1) AND
 C l(1) of EQ 5.

DATA ATZ/2*64.D1,641.6D0,27.D1/,ADZ/3*.319D0,1.55D0/,AAT/2*2.D4
 1,4.D4,25.D0/,AAD/34.D0,4.D1,3.D1,1.05D3/

DATA WM/18.0152D0/,GASCON/.461522D0/,TZ/647.073D0/,AA/1.D0/,NC/36/

DATA UREF,SREF/-4328.455039D0,7.6180802D0/

DATA G1,G2,GF/11.d0,44.3333333333333d0,3.5d0/

DATA P/.7478629,-.3540782,2*0.,.007159876,0.,-.003528426,3*0./

DATA Q/1.1278334,0.,-.5944001,-5.010996,0.,.63684256,4*0./

DATA G/- .53062968529023D3, .22744901424408D4, .78779333020687D3
 1,-.69830527374994D2, .17863832875422D5, -.39514731563338D5
 2, .33803884280753D5, -.13855050202703D5, -.25637436613260D6
 3, .48212575981415D6, -.34183016969660D6, .12223156417448D6
 4, .11797433655832D7, -.21734810110373D7, .10829952168620D7
 5, -.25441998064049D6, -.31377774947767D7, .52911910757704D7
 6, -.13802577177877D7, -.25109914369001D6, .46561826115608D7
 7, -.72752773275387D7, .41774246148294D6, .14016358244614D7
 8, -.31555231392127D7, .47929666384584D7, .40912664781209D6
 9, -.13626369388386D7, .69625220862664D6, -.10834900096447D7
 A, -.22722827401688D6, .38365486000660D6, .68833257944332D4
 B, .21757245522644D5, -.26627944829770D4, -.70730418082074D5
 C, -.225D0, -1.68D0, .055D0, -93.0D0/

DATA II/4*0,4*1,4*2,4*3,4*4,4*5,4*6,4*8,2*2,0,4,3*2,4/

DATA JJ/2,3,5,7,2,3,5,7,2,3,5,7,2,3,5,7,2,3,5,7,2,3,5,7
 1,2,3,5,7,1,3*4,0,2,0,0/

END


```

C      SUBROUTINE BB(T)
C      THIS SUBROUTINE CALCULATES THE B'S OF EQS. 3,4 USING COEFFICIENTS
C      FROM BLOCKDATA, CALCULATING ALSO THE FIRST AND SECOND DERIVS
C      W.R.TO TEMP. THE B'S CALCULATED HERE ARE IN CM3/G.
      implicit double precision(a-h,o-z)
      real p,q
      COMMON /ELLCON/ G1,G2,GF,B1,P2,P1T,B2T,B1TT,B2TT
      COMMON /ACONST/ WM,GASCON,TZ,AA,Z,DZ,Y,UREF,SREF
      COMMON /BCONST/ P(10),Q(10)
      DIMENSION V(10)
      V(1)=1.
      DO 2 I=2,10
2    V(I)=V(I-1)*TZ/T
      E1=P(1)+P(2)*ALOG(1./V(2))
      B2=Q(1)
      E1T=P(2)*V(2)/TZ
      B2T=0.
      B1TT=0.
      B2TT=0.
      DO 4 I=3,10
      B1=B1+P(I)*V(I-1)
      B2=B2+Q(I)*V(I-1)
      B1T=B1T-(I-2)*P(I)*V(I-1)/T
      B2T=B2T-(I-2)*Q(I)*V(I-1)/T
      B1TT=B1TT+P(I)*(I-2)**2*V(I-1)/T/T
4    B2TT=B2TT+Q(I)*(I-2)**2*V(I-1)/T/T
      B1TT=B1TT-E1T/T
      B2TT=B2TT-B2T/T
      RETURN
      END

```



```

C
C      SUBROUTINE BASE(D,T)
C This function calculates Z [=Pbase/(DRT) ] ,
C and also Abase,Gbase,Sbase,Ubase,Hbase,CVbase, AND 1/(DRT) * DP/DT
C for the base fct (called DPDTB)
C The AB,GB,SB,UB,HB and CVB are calculated in dimensionless units:
C AB/RT, GB/RT, SB/R, etc.
C      IMPLICIT REAL*8 (A-H,O-Z)
C      COMMON /ELLCON/ G1,G2,GF,B1,P2,B1T,B2T,B1TT,B2TT
C G1,G2 AND GF ARE THE ALPHA, BETA AND GAMMA OF EQ 2, WHICH ARE
C SUPPLIED BY THE BLOCKDATA ROUTINE. B1 AND P2 ARE THE "EXCLUDED
C VOLUME" AND "2ND VIRIAL" (EQS 3 AND 4) SUPPLIED BY THE SUBROUTINE
C BB(T), WHICH ALSO SUPPLIES THE 1ST AND 2ND DERIVATIVES WITH
C RESPECT TO T (B1T,B2T,B1TT,B2TT).
C      COMMON /BASEF/ AB,GB,SB,UB,HB,CVB,DPDTB
C      COMMON /ACONST/ WM,GASCON,TZ,A,Z,DZ,Y,UREF,SREF
C      Y=.25*B1*D
C      X=1.-Y
C      Z0=(1.+G1*Y+G2*Y*Y)/X**3
C      Z=Z0+4.*Y*(B2/B1-GF)
C      DZ0=(G1+2.*G2*Y)/X**3 + 3.*(1.+G1*Y+G2*Y*Y)/X**4
C      DZ=DZ0+4.*(P2/B1-GF)
C      AB = -DLOG(X)-(G2-1.)/X+28.16666667D0/X/X+4.*Y*(B2/B1-GF)
1 +15.166666667D0 + DLOG(D*T*4.55483D0)
C      GB = AB + Z
C      BB2TT=T*T*B2TT
C      UB= -T*B1T*(Z-1.-D*B2)/B1-D*T*B2T
C      HE=Z+UB
C      CVB=2.*UB+(Z0-1.)*((T*B1T/B1)**2-T*T*B1TT/B1)
1 - D*(BB2TT - GF*B1TT*T*T) -(T*B1T/B1)**2*Y*DZ0
C      DPDTB=Z/T + D*(DZ*B1T/4.+B2T-B2/B1*B1T)
C      SB = UB - AB
C      RETURN
C      END
C

```

C

SUBROUTINE QQ(T,D)

C THIS ROUTINE CALCULATES, FOR A GIVEN T(K) AND D(G/CM3), THE RESIDUAL
 C CONTRIBUTIONS TO: PRESSURE (Q), HELMHOLTZ FCT (AR), DP/DRHO (Q5),
 C AND ALSO TO THE GIBBS FUNCTION, ENTROPY, INTERNAL ENERGY, ENTHALPY,
 C ISOCHORIC HEAT CAPACITY AND DPDT. (EQ 5)
 C TERMS 37 THRU 39 ARE THE ADDITIONAL TERMS AFFECTING ONLY THE
 C IMMEDIATE VICINITY OF THE CRITICAL POINT, AND TERM 40 IS THE
 C ADDITIONAL TERM IMPROVING THE LOW T, HIGH P REGION.

IMPLICIT REAL*8(A-H,O-Z)

COMMON /RESF/ AR,GR,SR,UR,HR,CVR,DPDTR

COMMON /QQQQ/ Q,Q5

DIMENSION QR(11),QT(10),QZR(9),QZT(9)

EQUIVALENCE (QR(3),QZR(1)),(QT(2),QZT(1))

COMMON /NCONST/ G(40),II(40),JJ(40),N

COMMON /ACONST/ WM,GASCON,TZ,AA,Z,DZ,Y,UREF,SREF

COMMON /AEDCON/ ATZ(4),ADZ(4),AAT(4),AAD(4)

RT=GASCON*T

QR(1)=0.

Q5=0.

Q=0.D0

AR=0.D0

DADT=0.

CVR=0.

DPDTR=0.

E=DEXP(-AA*D)

Q10=D*D*E

Q20=1.D0-E

QR(2)=Q10

V=TZ/T

QT(1)=T/TZ

DO 4 I=2,10

QR(I+1)=QR(I)*Q20

4 QT(I)=QT(I-1)*V

DO 10 I=1,N

K=II(I)+1

L=JJ(I)

ZZ=K

QP=G(I)*AA*QZR(K-1)*QZT(L)

Q=Q+QP

Q5 = Q5 + AA*(2./D-AA*(1.-E*(K-1)/Q20))*QP

AR=AR+G(I)*QZR(K)*QZT(L)/Q10/ZZ/RT

DFDT=Q20**K*(1-L)*QZT(L+1)/TZ/K

D2F=L*DFDT

DPT=DFDT*Q10*AA*K/Q20

DADT=DADT+G(I)*DFDT

DPDTR=DPDTR+G(I)*DPT

10 CVR=CVR+G(I)*D2F/GASCON

QP=0.

Q2A=0.

C

```

DO 20 J=37,40
IF(G(J).EQ.0.D0) GO TO 20
K=II(J)
KM=JJ(J)
DDZ = ADZ(J-36)
DEL = D/DDZ - 1.
IF(DABS(DEL).LT.1.D-10) DEL=1.D-10
DD = DEL*DEL
EX1 = -AAD(J-36)*DEL**K
DEX=DEXP(EX1)*DEL**KM
ATT = AAT(J-36)
TX = ATZ(J-36)
TAU = T/TX-1.
EX2 = -ATT*TAU*TAU
TEX = DEXP(EX2)
Q10 = DEX*TEX
QM = KM/DEL - K*AAD(J-36)*DEL**(K-1)
FCT=QM*D**2*Q10/DDZ
Q5T = FCT*(2./D+QM/DDZ)-(D/DDZ)**2*Q10*(KM/DEL/DEL+
1 K*(K-1)*AAD(J-36)*DEL**(K-2))
Q5 = Q5 + Q5T*G(J)
QP = QP + G(J)*FCT
DADT = DADT - 2.*G(J)*ATT*TAU*Q10/TX
DPDTR = DPDTR - 2.*G(J)*ATT*TAU*FCT/TX
Q2A = Q2A + T*G(J)*(4.*ATT*EX2+2.*ATT)*Q10/TX/TX
AR = AR + Q10*G(J)/RT
20 CONTINUE
SR=-DADT/GASCON
UR=AR+SR
CVR=CVR+Q2A/GASCON
Q=Q+QP
RETURN
END

```

C

```

C      SUBROUTINE DFIND(DOUT,P,D,T,DPD)
C ROUTINE TO FIND DENSITY CORRESPONDING TO INPUT PRESSURE P(MPA), AND
C TEMPERATURE T(K), USING INITIAL GUESS DENSITY D(G/CM3). THE OUTPUT
C DENSITY IS IN G/CM3, ALSO, AS A BYPRODUCT, DP/DRHO IS CALCULATED
C ('DPD', MPA CM3/G)
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON /QQQQ/ Q0,Q5
      COMMON /ACONST/ WM,GASCON,TZ,AA,Z,DZ,Y,UREF,SREF
      DD=D
      RT=GASCON*T
      IF(DD.LE.0.) DD=1.D-8
      IF(DD.GT.1.9) DD=1.9
      L=0
9     L=L+1
11    IF(DD.LE.0.) DD=1.D-8
      IF(DD.GT.1.9) DD=1.9
      CALL BASE(DD,T)
      CALL QQ(T,DD)
      PP = RT*DD*Z + Q0
      DPD=RT*(Z+Y*DZ)+Q5
C THE FOLLOWING 3 LINES CHECK FOR NEGATIVE DP/DRHO, AND IF SO ASSUME
C GUESS TO BE IN 2-PHASE REGION, AND CORRECT GUESS ACCORDINGLY.
      IF(DPD.GT.0.D0) GO TO 13
      IF(D.GE..2967D0) DD=DD*1.02D0
      IF(D.LT..2967D0) DD=DD*.98D0
      IF(L.LE.10) GO TO 9
13    DPDX=DPD*1.1
      IF(DPDX.LT..1) DPDX=.1
      DP=DABS(1.-PP/P)
      IF(DP.LT.1.D-8) GO TO 20
      IF(D.GT..3 .AND. DP.LT.1.D-7) GO TO 20
      IF(D.GT..7 .AND. DP.LT.1.D-6) GO TO 20
      X=(P-PP)/DPDX
      IF(DABS(X).GT..1) X=X*.1/DABS(X)
      DD=DD+X
      IF(DD.LE.0.) DD=1.D-8
19    IF(L.LE.30) GO TO 9
20    CONTINUE
      DOUT=DD
      RETURN
      END

```

C

C

```

SUBROUTINE THERM(D,T)
IMPLICIT REAL*8(A-H,O-Z)
COMMON /ACONST/ WM,GASCON,TZ,AA,ZB,DZB,Y,UREF,SREF
COMMON /QQQQ/ QP,QDP
COMMON /BASEF/AB,GB,SB,UB,HB,CVB,DPDTB
COMMON /RESF/AR,GR,SR,UR,HR,CVR,DPDTR
COMMON /IDF/ AI,GI,SI,UI,HI,CVI,CPI
COMMON /FCTS/AD,GD,SD,UD,HD,CVD,CPD,DPDT,DVDT,CJTT,CJTH

```

C THIS SUBROUTINE CALCULATES THE THERMODYNAMIC FUNCTIONS IN
C DIMENSIONLESS UNITS (AD=A/RT, GD=G/RT, SD=S/R, UD=U/RT,
C HD=H/RT, CVD=CV/R, AND CPD=CP/R)

```

CALL IDEAL(T)
RT = GASCON*T
Z = ZB + QP/RT/D
DPDD = RT*(ZB+Y*DZB) + QDP
AD = AB + AR + AI - UREF/T + SREF
GD = AD + Z
UD = UB + UR + UI - UREF/T
DPDT = RT*D*DPDTB + DPDTR
CVD = CVB + CVR + CVI
CPD = CVD + T*DPDT**2/(D*D*DPDD*GASCON)
HD = UD + Z
SD = SE + SR + SI - SREF
DVDT=DPDT/DPDD/D/D
CJTT=1./D-T*DVDT
CJTH=-CJTT/CPD/GASCON
RETURN
END

```

C

```

FUNCTION PS(T)

```

C This function calculates an approximation to the vapor pressure, PS,
C as a function of the input temperature. The vapor pressure
C calculated agrees with the vapor pressure predicted by the surface
C to within .02% to within a degree or so of the critical temperature,
C and can serve as an initial guess for further refinement by
C imposing the condition that $G_l = G_v$.

```

IMPLICIT REAL*8 (A-H,O-Z)
DIMENSION A(8)/-7.8889166D0,2.5514255D0,-6.716169D0
1,33.239495D0,-105.38479D0,174.35319D0,-148.39348D0
2,48.631602D0/
IF(T.GT.314.D0) GO TO 2
PL=6.3573118D0-8858.843D0/T+607.56335D0*T**(-.6)
PS=.1*DEXP(PL)
RETURN
2 V=T/647.25D0
W=DABS(1.D0-V)
B=0.D0
DO 4 I=1,8
Z=I
4 B=B+A(I)*W**((Z+1.)/2.)
Q=B/V
PS=22.093D0*DEXP(Q)
RETURN
END

```

C

FUNCTION TSAT(P)

C This function calculates the saturation temperature for a given
 C pressure, by an iterative process using PSAT and TDPSDT.

REAL*8 P , PS , TG , TSAT,TDPSDT

TSAT=0.

IF(P.GT.22.05) RETURN

K=0

PL=2.302585*DLOG(P)

C PL=LOGE(10)*LOGE(P) TO CONVERT EQUATION FROM BARS TO MPa
 TG=372.83+PL*(27.7589+PL*(2.3819+PL*(.24834+PL*.0193855)))

1 IF(TG.LT.273.15) TG=273.15

IF(TG.GT.647.) TG=647.

IF(K.LT.8) GO TO 2

WRITE(6,3) K,P,PP,TG

3 FORMAT()

GO TO 8

2 K=K+1

PP=PS(TG)

DP=TDPSDT(TG)

IF(ABS(1.-PP/P).LT..00001) GO TO 8

TG = TG*(1.+(P-PP)/DP)

GO TO 1

8 TSAT=TG

RETURN

END

C

FUNCTION TDPSDT(T)

C This function calculates $T*(dPs/dT)$, and is used by the function TSAT.

IMPLICIT REAL*8 (A-H,O-Z)

DIMENSION A(8)/-7.8889166D0,2.5514255D0,-6.716169D0

1,33.239495D0,-105.38479D0,174.35319D0,-148.39348D0

2,48.631602D0/

V=T/647.25

W=1.-V

B=0.

C=0.

DO 4 I=1,8

Z=I

Y=A(I)*W**((Z+1.)/2.)

C=C+Y/W*(.5-.5*Z-1./V)

4 B=B+Y

Q=B/V

TDPSDT=22.093*DEXP(Q)*C

RETURN

END


```

C
C      SUBROUTINE IDEAL(T)
C      THIS SUBROUTINE CALCULATES THE THERMODYNAMIC PROPERTIES FOR
C      WATER IN THE IDEAL GAS STATE OF H.W. WOOLLEY
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON /IDF/ AI,GI,SI,UI,HI,CVI,CPI
      DIMENSION C(18)/.19730271018D2,.209662681977D2,-.483429455355D0
1,.605743189245D1,22.56023885D0,-9.87532442D0,-.43135538513D1
2,.458155781D0,-.47754901883D-1,.41238460633D-2,-.27929052852D-3
3,.14481695261D-4,-.56473658748D-6,.16200446D-7,-.3303822796D-9
4,.451916067368D-11,-.370734122708D-13,.137546068238D-15/
C      NOTE THAT THE TEMPERATURES ARE SCALED BY A FACTOR OF 100 HERE SO THAT
C      THE EXPONENT OF THE COEFFICIENT OF THE LAST TERM WILL BE WITHIN
C      RANGE FOR MOST COMPUTERS.
      TT=T/1.D2
      TL=DLOG(TT)
      GI=-(C(1)/TT+C(2))*TL
      HI=(C(2)+C(1)*(1.D0-TL)/TT)
      CPI=C(2)-C(1)/TT
      DO 8 I=3,18
      GI=GI-C(I)*TT**(I-6)
      HI=HI+C(I)*(I-6)*TT**(I-6)
8      CPI=CPI+C(I)*(I-6)*(I-5)*TT**(I-6)
      AI=GI-1.
      UI=HI-1.
      CVI=CPI-1.
      SI=UI-AI
      RETURN
      END
C
C      SUBROUTINE SECVIR(T,VIR)
C      THIS SUBROUTINE CALCULATES THE SECOND VIRIAL IN CM3/G
C      AT TEMPERATURE T IN K.
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON /NCONST/ G(40),II(40),JJ(40),NC
      COMMON /ELLCON/ G1,G2,GF,BB1,BB2,B1T,B2T,B1TT,B2TT
      COMMON /QQQQ/ Q0,Q5
      COMMON /ACONST/ WM,GASCON,TC,AA,Z,DZ,Y,UREF,SREF
      CALL BB(T)
      V=TC/T
      VIR=BB2
      DO 3 J=1,NC
      IF(II(J).NE.0) GO TO 3
      L=JJ(J)
      VIR=VIR+G(J)*V**(L-1)/T/GASCON
3      CONTINUE
      RETURN
      END

```

C

```

      SUBROUTINE CORR(T,P,DL,DV,DELG)
C SUBROUTINE CORR WILL CALCULATE, FOR AN INPUT T AND P AT OR
C VAPOR PRESSURE, THE CORRESPONDING LIQUID AND VAPOR DENSIT
C  $DELG = (GL-GV)/RT$  FOR USE IN CALCULATING THE CORRECTION T
C PRESSURE FOR  $DELG = 0$ .
      IMPLICIT DOUBLE PRECISION(A-H,O-Z)
      COMMON /QQQQ/ Q00,Q11
      COMMON /ACONST/ WM,GASCON,TZ,AA,ZB,DZB,YB,UREF,SREF
      COMMON /FCTS/ AD,GD,SD,UD,HD,CVD,CPD,DPDT,DVDT,CJTT,CJ
      DLIQ=DL
      IF(DL.LE.0.) DLIQ=1.11-.0004*T
      CALL EB(T)
      RT=GASCON*T
      CALL DFIND(DL,P,DLIQ,T,DQ)
      CALL THERM(DL,T)
      GL=GD
      DVAP=DV
      IF(DV.LE.0.) DVAP=P/GASCON/T
      CALL DFIND(DV,P,DVAP,T,DQ)
      IF(DV.LT.5.D-7) DV=5.D-7
      CALL THERM(DV,T)
      GV=GD
      DELG = GL-GV
      RETURN
      END

```

CC

```

      SUBROUTINE PCORR(T,P,DL,DV)
C SUBROUTINE PCORR WILL CALCULATE THE VAPOR PRESSURE P AND T
C VAPOR DENSITIES CORRESPONDING TO THE INPUT T, CORRECTED S
C  $GL-GV=0$ . THE FUNCTION PS IS REQUIRED WHICH WILL GIVE A R
C GOOD APPROXIMATION TO THE VAPOR PRESSURE TO BE USED AS TH
C POINT FOR THE ITERATION.
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      COMMON /ACONST/ WM,GASCON,TZ,AA,ZB,DZB,YB,UREF,SREF
      P = PS(T)
2    CALL CORR(T,P,DL,DV,DELG)
      DP=DELG*GASCON*T/(1./DV-1./DL)
      P = P+DP
      IF(DABS(DELG).LT.1.D-4) RETURN
      GOTO 2
      END

```

CC

```

      SUBROUTINE TCCORR(T,P,DL,DV)
C SUBROUTINE TCCORR IS SIMILAR TO "PCORR" EXCEPT THAT THE TEM
C CORRESPONDING TO THE INPUT VAPOR PRESSURE IS FOUND. FUNCT
C ARE TSAT AND TDPSDT WHICH GIVE AN APPROXIMATION TO T(SAT)
C  $T*DP(SAT)/DT$ .
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      COMMON /ACONST/ WM,GASCON,TZ,AA,ZB,DZB,YB,UREF,SREF
      T = TSAT(P)
2    CALL CORR(T,P,DL,DV,DELG)
      DP=DELG*GASCON*T/(1./DV-1./DL)
      T = T*(1.-DP/TDPSDT(T))
      IF(DABS(DELG).LT.1.D-4) RETURN
      GO TO 2
      END

```

```

C
c The following 3 subroutines form a package allowing the us
c   operate in a system of units of his choice.
  SUBROUTINE UNIT
C THIS SUBROUTINE QUERIES THE USER AS TO HIS CHOICE OF UNITS
C   INTERNAL PARAMETERS APPROPRIATELY.  THE INTERNAL UNITS OF
C   TEMPERATURES IN K, DENSITIES IN G/CM3, ALL OTHER QUANTITI
C   IN DIMENSIONLESS UNITS AND DIMENSIONED AT OUTPUT TIME.
  IMPLICIT DOUBLE PRECISION (A-H,O-Z)
  DOUBLE PRECISION NT,ND,NP,NH,NNT,NND,NNP,NNH
  COMMON /UNITS/ IT,ID,IP,IH,NT,ND,NP,NH,FT,FD,FP,FH
  DIMENSION FFD(4),FFP(5),FFH(6),NNT(4),NND(4),NNP(5),NN
  DATA FFD/1.D-3,1.D0,.0180152D0,.016018D0/
  DATA FFP/1.D0,10.D0,9.869232667D0,145.038D0,10.1971D0/
  DATA FFH/2*1.D0,18.0152D0,.23884590D0,4.30285666D0,.42
  DATA NNT/1HK,1HC,1HR,1HF/
  DATA NND/6Hkg/m3 ,6Hg/cm3 ,6Hmol/L ,6Hlb/ft3/
  DATA NNP/6H MPa ,6H Bar ,6H Atm ,6H PSI ,6Hkg/cm2/
  DATA NNH/6HkJ/kg ,6H J/g ,6HJ/mol ,6Hcal/g ,7Hcal/mol
  DATA A1,A2,A3,A4/8HTEMPERAT,7HDENSITY
1,8HPRESSURE, 8HENERGY /
  WRITE(6,11) A1
30  WRITE(6,12)
  READ(5,10,END=99) IT
  IF(IT.EQ.0) STOP
  IF(IT.GT.4) GOTO 30
  NT=NNT(IT)
  WRITE(6,11) A2
31  WRITE(6,13)
  READ(5,10,END=99) ID
  IF(ID.GT.4 .OR. ID.LT.1) GOTO 31
  ND=NND(ID)
  FD=FFD(ID)
  WRITE(6,11) A3
32  WRITE(6,14)
  READ(5,10,END=99) IP
  IF(IP.GT.5 .OR. IP.LT.1) GOTO 32
  NP=NNP(IP)
  FP=FFP(IP)
  WRITE(6,11) A4
33  WRITE(6,15)
  READ(5,10,END=99) IH
  IF(IH.GT.6 .OR. IH.LT.1) GOTO 33
  NH=NNH(IH)
  FH=FFH(IH)
  RETURN
99  STOP
10  FORMAT()
11  FORMAT(' ENTER UNITS CHOSEN FOR ',A8)
12  FORMAT(' CHOOSE FROM 1=DEG K, 2=DEG C, 3=DEG R, 4=DEG
13  FORMAT(' CHOOSE FROM 1=KG/M3, 2=G/CM3, 3=MOL/L, 4=LB/F
14  FORMAT(' CHOOSE FROM 1=MPA, 2=BAR, 3=ATM, 4=PSIA, 5=KG
15  FORMAT(' CHOOSE FROM 1=KJ/KG, 2=J/G, 3=J/MOL, 4=CALORI
1RIES/MOL, 6=BTU/LB')
  END

```

C

FUNCTION TTT(T)

C FUNCTION TO CONVERT INPUT TEMPERATURES IN EXTERNAL UNITS T

DOUBLE PRECISION T,TTT,FT,FD,FP,FH,NT,ND,NP,NH

COMMON /UNITS/ IT,ID,IP,IH,NT,ND,NP,NH,FT,FD,FP,FH

GO TO (1,2,3,4),IT

1 TTT=T

FT=1.

RETURN

2 TTT=T+273.15D0

FT=1.

RETURN

3 TTT=T/1.8D0

FT=.55555555555556D0

RETURN

4 TTT=(T+459.67D0)/1.8D0

FT=.55555555555556D0

RETURN

END

FUNCTION TTI(T)

C FUNCTION TO CONVERT INTERNAL TEMPERATURES IN DEG K TO EXTE

DOUBLE PRECISION T,TTI,FT,FD,FP,FH,NT,ND,NP,NH

COMMON /UNITS/ IT,ID,IP,IH,NT,ND,NP,NH,FT,FD,FP,FH

GO TO (5,6,7,8),IT

5 TTI=T

RETURN

6 TTI=T-273.15D0

RETURN

7 TTI=T*1.8D0

RETURN

8 TTI=T*1.8D0-459.67D0

RETURN

END

APPENDIX B

This appendix contains sample calculations to help the user test his program. Also listed are the main programs used to print out numerical values.

```

C THIS IS A MAIN PROGRAM FOR THE CALCULATION OF TABLES OF PROPERTIES
C USING A CHOICE OF UNITS, AND AT A CHOICE OF CONSTANT TEMPERATURE,
C PRESSURE OR DENSITY. THE USER IS QUERIED AS TO HIS CHOICES OF
C UNITS AND VARIABLES AT EXECUTION TIME.
  IMPLICIT DOUBLE PRECISION(A-H,O-Z)
  DOUBLE PRECISION NT,ND,NP,NH
  COMMON /UNITS/ IT,ID,IP,IH,NT,ND,NP,NH,FT,FD,FP,FH
  COMMON /QQQQ/ Q0,Q5
  COMMON /FCTS/ AD,GD,SD,UD,HD,CVD,CPD,DPDT
  COMMON /ACONST/ WM,GASCON,TC,AA,Z,DZ,Y,UREF,SREF
  COMMON /NCONST/ G(40),II(40),JJ(40),NC
  DATA NS1,NS2/2H m,2Hft/
  CALL UNIT
  NS=NS1
  IF(ID.EQ.4) NS=NS2
15  WRITE(6,11)
  READ(5,*,END=9) IOPT,XISO
  IF(IOPT.EQ.0) GO TO 9
  GO TO (101,201,301),IOPT
101 WRITE(6,102)
102 FORMAT(' ENTER OTHER INDEPENDENT VARIABLE (2 FOR P, 3 FOR DENS'/
1' FOLLOWED BY INITIAL, FINAL AND INCREMENTAL VALUES OF THIS VAR.')
  READ(5,*,END=9) JOPT,Y1,Y2,YI
  IF(JOPT-1) 15,101,103
103 TT=XISO
  T=TTT(TT)
  WRITE(6,444) NT,NP,ND,NP,NT,NH,NT,NH,NS
  IF(JOPT.EQ.2) DGSS=Y1/FP/T/.4
  IZ=0
  CALL BB(T)
  PSS=200000.
  DVV=0.
  IF(T.LT.TC) CALL PCORR(T,PSS,DLL,DVV)
  DGSS=DVV
  IF(DGSS.EQ.0.) DGSS=1.11-.0004*T
  PSAT=PSS*FP
  IF(JOPT.EQ.2 .AND. Y1.GT.PSAT) IZ=3
  IF(Y1.GT.PSAT) DGSS=DLL
  IF(JOPT.GE.3) IZ=3
  PIN=Y1-YI
  DIN=PIN
  PINC=YI/FP
  DINC=YI*FD
22 IF(JOPT.EQ.2) PIN=PIN+YI
  IF(JOPT.EQ.3) DIN=DIN+YI
  IF(JOPT.EQ.2 .AND. PIN.GT.Y2) GO TO 101
  IF(JOPT.EQ.3 .AND. DIN.GT.Y2) GO TO 101
  IF(JOPT.EQ.2) PRES=PIN/FP
  IF(JOPT.EQ.3) D=DIN/FD
24 CONTINUE

```



```

IF(JOPT.EQ.3 .OR. (JOPT.EQ.2 .AND. PIN.LT.PSAT)) GO TO 26
IF(JOPT.EQ.1 .AND. T.LT.TS) GO TO 26
TSAVE=TT-YI
IF(JOPT.EQ.1 .AND. IOPT.EQ.2 .AND. IZ.LE.2) TT=TTI(TS)
PSAVE=PIN-YI
IF(JOPT.EQ.2 .AND. PRES.GT.PSAT/FP .AND. IZ.GE.2) GO TO 26
IF(JOPT.EQ.1 .AND. T.GT.TS .AND. IZ.GE.2) GO TO 26
23 IZ=IZ+1
IF(JOPT.EQ.2) PRES=PSAT/FP
IF(JOPT.EQ.1) T=TS
IF(IZ.EQ.1 .AND. JOPT.EQ.1) DGSS=DLL
IF(IZ.EQ.1 .AND. JOPT.EQ.2) DGSS=DVV
IF(IZ.EQ.2 .AND. JOPT.EQ.2) DGSS=DLL
IF(IZ.EQ.2 .AND. JOPT.EQ.1) DGSS=DVV
CALL EB(T)
26 IF(IOPT.NE.3 .AND. JOPT.NE.3) CALL DFIND(D,PRES,DGSS,T,DQ)
27 CALL QQ(T,D)
CALL BASE(D,T)
RT=GASCON*T
PDUM = D*RT*Z + Q0
IF(JOPT.EQ.3 .OR. IOPT.EQ.3) PRES=PDUM
IF(IOPT.EQ.3 .OR. JOPT.EQ.3) DQ=RT*(Z+Y*DZ)+Q5
DGSS=D + PINC/DQ
CALL THERM(D,T)
U = UD*T*GASCON*FH
C=DSQRT(DABS(CPD*DQ*1.D3/CVD))
IF(ID.EQ.4) C=C*3.280833
H = HD*T*GASCON*FH
S = SD*GASCON*FH*FT
dpdtx=dpdt*fp*ft
dpdd=dq*fp*fd
COMP = 1.E3/D/DQ/FP
DDDTL=1.D3*DPDT/D/DQ
CP=CPD*GASCON*FH*FT
CV=CVD*GASCON*FH*FT
VL=fd/D
DOUT=1./VL
POUT=PRES*FP
WRITE(6,21) TT,POUT,DOUT,DPDTX,DPDD,CV,CP,S,H,U,C
21 FORMAT(F9.3,F12.5,F12.7,F11.5,F11.3,5F12.4,F11.3)
444 FORMAT(5X,1HT,12X,1HP,10X,1HD,8X,5HdP/dT,5X,5HdP/dD,10X,2HCv
1,10X,2HCp,11X,1HS,9X,1HH,11X,1HU,7X,7HVel Snd/3X,4Hdeg ,A1,7X,A8
2,4X,A6,5X,A3,1H/,A1,4X,7H ,15X,4H- - ,A6,A1,4H - -
3,13X,4H- - ,A6,4H - -,8X,A2,4H/sec/)
11 FORMAT( ' DO YOU WISH TO CALCULATE AN ISOTHERM (ENTER 1), AN ISOBA
1R (ENTER 2) OR AN ISOCHORE? (ENTER 3)'' FOLLOWED BY VALUE OF ISO.
2 (ENTER 0 TO DISCONTINUE)')
IF(IZ.EQ.1) WRITE(6,12)
12 FORMAT(' -----
1-----')

```

```

      IF(IZ.EQ.1) GO TO 23
      IF(IZ.EQ.2 .AND. JOPT.EQ.2) PIN=PSAVE
      IF(IZ.EQ.2 .AND. JOPT.EQ.1) TT=TSAVE
      IF(IZ.EQ.2) IZ = 3
      GO TO (22,204,304),IOPT
201  JOPT=1
      PRES = XISO/FP
202  WRITE(6,203)
203  FORMAT(' ENTER FIRST LAST AND INCREMENT OF T')
      READ(5,*,END=9) T1,T2,YI
      IF(T1.EQ.0.) GO TO 15
      WRITE(6,444) NT,NP,ND,NP,NT,NH,NT,NH,NS
      TT=T1-YI
      T=TTT(TT)
      CALL TCORR(TS,PRES,DLL,DVV)
      D = DLL
      IF((T+YI*FT).GT.TS) D=DVV
      IZ=3
      IF((T+YI*FT).LT.TS) IZ=0
204  TT=TT+YI
      T=TTT(TT)
      IF(TT.GT.T2) GO TO 202
      CALL BB(T)
      DGSS=D
      GO TO 24
301  JOPT=1
      D=XISO
302  WRITE(6,203)
      READ(5,*,END=9) T1,T2,YI
      IF(T1.LE.0.) GO TO 15
      WRITE(6,444) NT,NP,ND,NP,NT,NH,NT,NH,NS
      TT=T1-YI
      IZ=3
      T=TTT(TT)
304  TT=TT+YI
      T=TTT(TT)
      IF(TT.GT.T2) GO TO 302
      CALL BB(T)
      GO TO 27
9      STOP
      END

```

```

C THE FOLLOWING IS A MAIN PROGRAM FOR CALCULATING THE PROPERTIES
C ALONG THE SATURATION CURVE UP TO 646.3 K. THE INPUTS ARE: INITIAL T,
C FINAL T AND THE T INCREMENT (ALL IN K). THE VAPOR PRESSURE IS FIRST
C CALCULATED USING "PS" AND ADJUSTED FROM THERE SO THAT
C  $GL-GV=0$ . ALSO IN THE INPUT ARE AN INITIAL GUESS FOR THE LIQUID AND
C VAPOR DENSITIES. IF NOT GIVEN, THEY WILL BE INTERNALLY CHOSEN.
  IMPLICIT REAL*8 (A-H,O-Z)
  COMMON /ACONST/ WM,GASCON,TZ,AA,ZB,DZB,YB
  COMMON /FCTS/ AD,GD,SD,UD,HD,CVD,CPD,DPDT
3  READ(5,4,END=99) TI,TF,TD,DL,DG
4  FORMAT()
  WRITE(6,22)
  T=TI-TD
6  T=T+TD
  IF(T.GT.TF) GO TO 3
  IF(T.GT.646.3D0) GO TO 3
  IJK=0
  CALL BB(T)
  P=PS(T)+IJK*PT
C THE FOLLOWING TWO LINES CALCULATE AN INITIAL GUESS FOR THE DENSITIES
C IF GUESSES NOT SUPPLIED IN THE INPUT.
  IF(DL.LE.0.) DL=1.11-.0004*T
  IF(DG.LE.0.) DG=P/GASCON/T
5  P=P+IJK*PT
  RT=GASCON*T
  CALL DFIND(RL,P,DL,T,DPDL)
  DL=RL
  CALL THERM(RL,T)
  SL=SD*GASCON
  HL = HD*GASCON*T
  VL=1./DL
  GL=GD
  CALL DFIND(RG,P,DG,T,DPDG)
  DG=RG
  IF(RG.LT.5.D-7) RG=5.D-7
  CALL THERM(RG,T)
  SG=SD*GASCON
  HG = HD*GASCON*T
  VG=1./DG
  GV=GD
  HEAT=HG-HL
  DELG=GL-GV
  IF(DABS(DELG).LT.2.D-6) GOTO 15
  PT = DELG*GASCON*T/(VG-VL)
  IF(T.GT.640.D0) PT=.1*PT
  IJK=IJK+1
  IF(IJK.EQ.1 .OR. (T.GT.64.D1 .AND. IJK.LE.10)) GO TO 5
15 HEAT=HG-HL
  WRITE(6,21) T,P,RL,RG,HL,HG,HEAT,SL,SG,VL,VG
21  FORMAT(F9.3,F13.6,F9.6,F9.7,3F9.2,2F9.4,F9.5,F11.3)
22  FORMAT('      T,K          P,MPA      DL,G/CC  DV,G/CC  HL,J/G  HV,J/G
1  LAT HT      SL,J/GK  SV,J/GX      VL      VG'/)
  GO TO 6
99  STOP
  END

```

C THIS IS A SAMPLE MAIN PROGRAM WHICH WILL SERVE AS AN EXAMPLE FOR
 C THE USE OF THE SUBROUTINES AND FUNCTIONS GIVEN ABOVE, AND WHICH
 C WILL PRINT OUT VALUES OF VARIOUS PROPERTIES CALCULATED FOR A
 C GIVEN INPUT POINT TO A LARGE NUMBER OF SIGNIFICANT FIGURES,
 C SUITABLE FOR USE AS A CHECK ON THE OPERATION OF THE PROGRAM.
 C THE USER IS QUERIED AS TO THE UNITS DESIRED.

```

    IMPLICIT DOUBLE PRECISION(A-H,O-Z)
    DOUBLE PRECISION NT,ND,NP,NH
    COMMON /UNITS/ IT,ID,IP,IH,NT,ND,NP,NH,FT,FD,FP,FH
    COMMON /QQQQ/ Q0,Q5
    COMMON /FCTS/ AD,GD,SD,UD,HD,CVD,CPD,DPDT,DVDT,CJTT,CJTH
    COMMON /ACONST/ WM,GASCON,TZ,AA,Z,DZ,Y,UREF,SREF
    COMMON /NCONST/ G(40),II(40),JJ(40),NC
    DATA NSS1,NSS2/2H m,2Hft/
    CALL UNIT
    NS=NSS1
    IF(ID.EQ.4) NS=NSS2
15  WRITE(6,11)
100 READ(5,*,END=9) IOPT,X,TT
    T=TTT(TT)
    RT=GASCON*T
    CALL BB(T)
    IF(IOPT.LE.0) GOTO 9
    GOTO (101,102,100,100,100),IOPT
101 DD=X
    D=DD*FD
    CALL CQ(T,D)
    CALL BASE(D,T)
    PRES = FP*(RT*D*Z + Q0)
    DQ=RT*(Z+Y*DZ)+Q5
    GOTO 111
102 PRES=X
    P=PRES/FP
    DGSS=P/T/.4
    PSAT=20000.
    IF(T.LT.TZ) CALL PCORR(T,PSAT,DLL,DGSS)
    IF(P.GT.PSAT) DGSS=DLL
    IF(P.GE.PSAT .AND. T.LT.523.15) DGSS=1.11-.0004*T
    CALL DFIND(D,P,DGSS,T,DQ)
    DD=D/FD
111 CALL THERM(D,T)
    U = UD*T*GASCON*FH
    C=DSORT(DABS(CPD*DQ*1.D3/CVD))
    IF(ID.EQ.4) C=C*3.280833
    H = HD*T*GASCON*FH
    S = SD*GASCON*FH*FT
    CP=CPD*GASCON*FH*FT
    CV=CVD*GASCON*FH*FT
    VL=1./D
    DPDD = DQ*FD*FP
    DPDT1=DPDT*FP*FT
    WRITE(6,20) TT,NT,PRES,NF,DD,ND

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```

WRITE(6,21) DPDT1,DPDD,CV,NH,NT,CP,S,H,NH,U,C,NS,CJTT,CJTH,DVDT
20 FORMAT(' T =',F12.4,' deg ',A1,5X,' P =',F13.6,1X,A6,5X,' D =',
1,F14.10,1X,A8)
21 FORMAT(' DP/DT =',F16.9,6X,' DP/DD =',F16.5/
2 ' CV =',F12.6,1X,A6,A1,5X,' CP =',F12.6,6X,' S =',F12.6/
3 ' H =',F14.6,1X,A6,5X,' U =',F14.6,6X,' VEL SND =',F14.6,A2,'/sec'/
4 ' JT(T) =',F11.5,5X,' JT(H) =',F11.5,5X,' DV/DT =',F12.6/)
11 FORMAT(' ENTER OPTION, X, AND T, WHERE FOR OPTION=1, X=DENSITY'/
1 ' AND FOR OPTION=2, X=PRESSURE (ENTER 0 TO QUIT)')
GO TO 100
9 STOP
END

```

NEXT POINT

ENTER UNITS CHOSEN FOR TEMPERAT

CHOOSE FROM 1=DEG K, 2=DEG C, 3=DEG R, 4=DEG F

>1

ENTER UNITS CHOSEN FOR DENSITY

CHOOSE FROM 1=KG/M3, 2=G/CM3, 3=MOL/L, 4=LB/FT3

>2

ENTER UNITS CHOSEN FOR PRESSURE.

CHOOSE FROM 1=MPA, 2=BAR, 3=ATM, 4=PSIA, 5=KG/CM2

>2

ENTER UNITS CHOSEN FOR ENERGY

CHOOSE FROM 1=KJ/KG, 2=J/G, 3=J/MOL, 4=CALORIES/G, 5=CALORIES/MOL, 6=BTU/LB

>2

ENTER OPTION, X, AND T, WHERE FOR OPTION=1, X=DENSITY

AND FOR OPTION=2, X=PRESSURE (ENTER 0 TO QUIT)

>1, .9, 873.15

T =	873.1500 deg K	P =	7110.805028 Bar	D =	.9000000000 g/cm3
DP/DT =	14.491600834	DP/DD =	28719.49752		
CV =	2.827220 J/g K	CP =	3.615462	S =	4.064690
H =	2779.151751 J/g	U =	1989.062303	VEL SND =	1916.419293 m/sec
JT(T) =	.56718	JT(H) =	-.15688	DV/DT =	.000623

>2, 225., 648.15

T =	648.1500 deg K	P =	225.000000 Bar	D =	.4103745556 g/cm3
DP/DT =	3.447888683	DP/DD =	63.95378		
CV =	3.743787 J/g K	CP =	75.284775	S =	4.221788
H =	1965.692198 J/g	U =	1910.864237	VEL SND =	358.617190 m/sec
JT(T) =	-205.05536	JT(H) =	2.72373	DV/DT =	.320130

>2, .00617, 273.16

T =	273.1600 deg K	P =	.006170 Bar	D =	.9997782189 g/cm3
DP/DT =	-1.576872063	DP/DD =	19608.40085		
CV =	4.225225 J/g K	CP =	4.228690	S =	.000000
H =	.000617 J/g	U =	-.000000	VEL SND =	1400.874132 m/sec
JT(T) =	1.02220	JT(H) =	-.24173	DV/DT =	-.000080

>

T deg C	P MPa	D g/cm ³	V cm ³ /g
50.000	.0100	.000067	14869.238335
50.000	.0123	.000083	12036.663719

50.000	.0123	.987991	1.012155
50.000	.1000	.988030	1.012116
50.000	1.0000	.988422	1.011713
50.000	10.0000	.992305	1.007754
50.000	20.0000	.996526	1.003486
50.000	30.0000	1.000656	.999344
50.000	40.0000	1.004700	.995322
50.000	50.0000	1.008663	.991411
50.000	60.0000	1.012550	.987605
50.000	70.0000	1.016365	.983899
50.000	80.0000	1.020109	.980287
50.000	90.0000	1.023788	.976765
50.000	100.0000	1.027403	.973328
50.000	200.0000	1.060447	.942999
50.000	300.0000	1.088794	.918448
50.000	400.0000	1.113570	.898013
50.000	500.0000	1.135810	.880429
50.000	600.0000	1.156346	.864793
50.000	700.0000	1.175655	.850590
50.000	800.0000	1.193766	.837685
50.000	900.0000	1.210356	.826203
50.000	1000.0000	1.225100	.816260

T deg C	P MPa	D g/cm ³	V cm ³ /g
250.000	.0100	.000041	24136.161956
250.000	.1000	.000416	2406.053164
250.000	1.0000	.004298	232.644926
250.000	3.9736	.019956	50.110581

250.000	3.9736	.799072	1.251452
250.000	10.0000	.805899	1.240850
250.000	20.0000	.816284	1.225064
250.000	30.0000	.825733	1.211046
250.000	40.0000	.834438	1.198411
250.000	50.0000	.842537	1.186892
250.000	60.0000	.850128	1.176293
250.000	70.0000	.857288	1.166469
250.000	80.0000	.864075	1.157307
250.000	90.0000	.870537	1.148717
250.000	100.0000	.876711	1.140627
250.000	200.0000	.927623	1.078024
250.000	300.0000	.966827	1.034311
250.000	400.0000	.999498	1.000502
250.000	500.0000	1.027884	.972872
250.000	600.0000	1.053194	.949493
250.000	700.0000	1.076161	.929229
250.000	800.0000	1.097271	.911352
250.000	900.0000	1.116861	.895367
250.000	1000.0000	1.135179	.880918

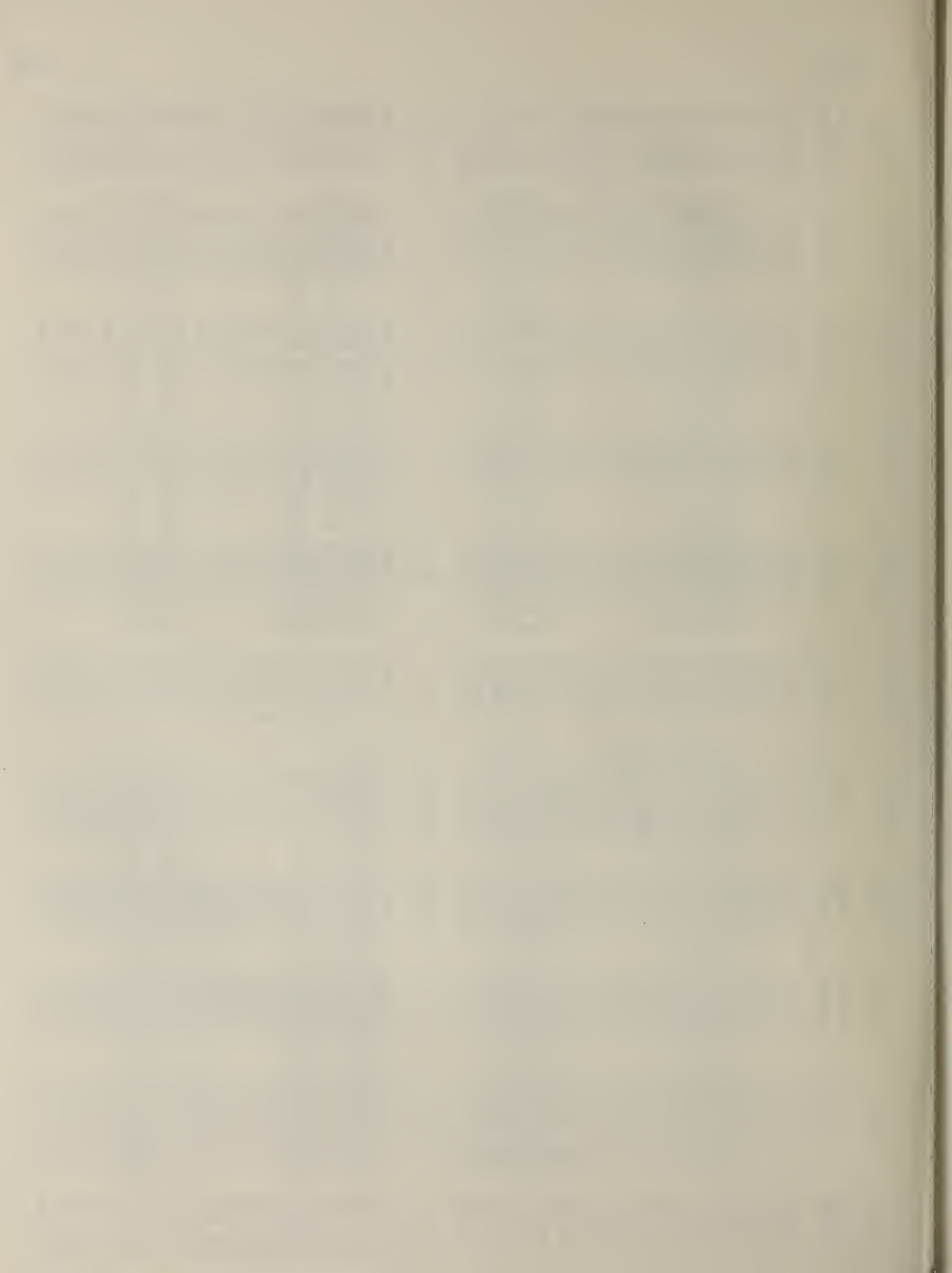
T deg C	P MPa	D g/cm ³	V cm ³ /g
375.000	.0100	.000033	29909.055417
375.000	.1000	.000335	2986.855135
375.000	1.0000	.003395	294.567937
375.000	10.0000	.040763	24.532263
375.000	20.0000	.130420	7.667535
375.000	22.3292	.320009	3.124909
375.000	30.0000	.558254	1.791298
375.000	40.0000	.609556	1.640537
375.000	50.0000	.641323	1.559276
375.000	60.0000	.665164	1.503388
375.000	70.0000	.684567	1.460777
375.000	80.0000	.701090	1.426350
375.000	90.0000	.715576	1.397475
375.000	100.0000	.728535	1.372617
375.000	200.0000	.816920	1.224110
375.000	300.0000	.873641	1.144634
375.000	400.0000	.917244	1.090222
375.000	500.0000	.953396	1.048882
375.000	600.0000	.984657	1.015582
375.000	700.0000	1.012420	.987732
375.000	800.0000	1.037537	.963821
375.000	900.0000	1.060570	.942869
375.000	1000.0000	1.081910	.924291

T deg C	P MPa	D g/cm ³	V cm ³ /g
500.000	.0100	.000028	35679.867768
500.000	.1000	.000280	3565.549685
500.000	1.0000	.002824	354.099874
500.000	10.0000	.030503	32.783626
500.000	20.0000	.067711	14.768678
500.000	30.0000	.115259	8.676122
500.000	40.0000	.177974	5.618801
500.000	50.0000	.256947	3.891860
500.000	60.0000	.338443	2.954707
500.000	70.0000	.405762	2.464496
500.000	80.0000	.456993	2.188216
500.000	90.0000	.496532	2.013967
500.000	100.0000	.528211	1.893181
500.000	200.0000	.691177	1.446808
500.000	300.0000	.772885	1.293853
500.000	400.0000	.830456	1.204158
500.000	500.0000	.876029	1.141515
500.000	600.0000	.914303	1.093730
500.000	700.0000	.947615	1.055281
500.000	800.0000	.977308	1.023219
500.000	900.0000	1.004227	.995791
500.000	1000.0000	1.028941	.971873

T deg C	P MPa	D g/cm ³	V cm ³ /g
750.000	.0100	.000021	47219.519942
750.000	.1000	.000212	4720.958893
750.000	1.0000	.002123	471.103828
750.000	10.0000	.021679	46.127641
750.000	20.0000	.044390	22.527645
750.000	30.0000	.068163	14.670731
750.000	40.0000	.092985	10.754408
750.000	50.0000	.118770	8.419621
750.000	60.0000	.145340	6.880435
750.000	70.0000	.172425	5.799609
750.000	80.0000	.199697	5.007588
750.000	90.0000	.226804	4.409089
750.000	100.0000	.253421	3.946003
750.000	200.0000	.462110	2.163988
750.000	300.0000	.584047	1.712190
750.000	400.0000	.665974	1.501561
750.000	500.0000	.728216	1.373220
750.000	600.0000	.779010	1.283680
750.000	700.0000	.822326	1.216062
750.000	800.0000	.860356	1.162309
750.000	900.0000	.894435	1.118025
750.000	1000.0000	.925435	1.080573

T deg C	P MPa	D g/cm ³	V cm ³ /g
1000.000	.0100	.000017	58758.280969
1000.000	.1000	.000170	5875.475023
1000.000	1.0000	.001703	587.198410
1000.000	10.0000	.017122	58.404407
1000.000	20.0000	.034420	29.052786
1000.000	30.0000	.051866	19.280576
1000.000	40.0000	.069439	14.401171
1000.000	50.0000	.087117	11.478860
1000.000	60.0000	.104867	9.535858
1000.000	70.0000	.122648	8.153425
1000.000	80.0000	.140405	7.122229
1000.000	90.0000	.158081	6.325872
1000.000	100.0000	.175613	5.694349
1000.000	200.0000	.333285	3.000438
1000.000	300.0000	.451565	2.214522
1000.000	400.0000	.539879	1.852267
1000.000	500.0000	.609226	1.641426
1000.000	600.0000	.666407	1.500584
1000.000	700.0000	.715338	1.397941
1000.000	800.0000	.758357	1.318641
1000.000	900.0000	.796939	1.254801
1000.000	1000.0000	.832065	1.201830

T deg C	P MPa	D g/cm ³	dP/dT MPa/C	dP/dD	Cv	Cp J/g	S	H J/g	U	Vel Snd m/sec
50.000	0.01000	0.00067	0.00031	148.242	1.43653	1.91016	8.17313	2591.753	2443.061	443.950
50.000	0.01234	0.00083	0.00039	149.028	1.44287	1.91942	8.07451	2591.191	2442.604	443.756
50.000	0.01234	0.00091	1.002431	2287.759	4.72713	4.18167	7.0774	209.327	209.315	1541.283
50.000	0.01000	0.00230	1.003659	2288.246	4.72690	4.18147	7.07370	209.403	209.301	1541.453
50.000	1.00000	0.00422	1.0036005	2293.242	4.02461	4.17942	7.0328	210.179	209.167	1543.195
50.000	10.00000	0.002305	1.0059519	2342.418	4.02224	4.15952	6.9914	217.926	207.849	1562.278
50.000	20.00000	0.00526	1.005811	2395.576	3.97843	4.13858	6.9456	226.523	226.433	1576.610
50.000	30.00000	0.00656	1.112335	2447.431	3.95566	4.11882	6.9091	235.046	205.066	1595.753
50.000	40.00000	1.004700	1.139128	2498.218	3.93387	4.10015	6.8548	243.556	203.743	1613.534
50.000	50.00000	1.008663	1.166209	2548.145	3.91300	4.08253	6.8097	252.033	202.462	1630.503
50.000	60.00000	1.012550	1.193590	2597.395	3.89300	4.06588	6.7548	260.477	201.221	1647.039
50.000	70.00000	1.016365	1.221230	2646.133	3.87383	4.05014	6.7201	268.889	200.015	1663.301
50.000	80.00000	1.020109	1.249140	2694.503	3.85545	4.03527	6.6754	277.268	198.848	1679.339
50.000	90.00000	1.023788	1.277278	2742.633	3.83782	4.02121	6.6310	285.615	197.726	1695.197
50.000	100.00000	1.027403	1.305609	2790.636	3.82091	4.00791	6.5866	293.931	196.599	1710.510
50.000	200.00000	1.060447	1.599278	3279.014	3.68512	3.90648	6.1497	375.549	186.952	1864.396
50.000	300.00000	1.088794	1.847577	3790.663	3.59236	3.83763	5.7274	454.958	179.424	2012.383
50.000	400.00000	1.113570	2.083891	4283.281	3.52256	3.78717	5.3264	532.794	173.599	2145.812
50.000	500.00000	1.135810	2.357987	4700.461	3.46653	3.76283	4.9375	609.131	168.917	2258.617
50.000	600.00000	1.156346	2.754523	5030.355	3.42196	3.78648	4.5408	683.546	164.672	2359.282
50.000	700.00000	1.175655	3.333416	5335.256	3.39432	3.88125	4.1110	755.428	160.016	2469.944
50.000	800.00000	1.193766	4.073168	5741.012	3.38910	4.04441	3.6352	824.454	154.306	2617.457
50.000	900.00000	1.210356	4.847013	6369.168	3.40483	4.21850	3.1236	891.103	147.520	2809.132
50.000	1000.00000	1.225100	5.486680	7255.468	3.43073	4.32406	2.6099	956.583	140.323	3024.027
T deg C	P MPa	D g/cm ³	dP/dT MPa/C	dP/dD	Cv	Cp J/g	S	H J/g	U	Vel Snd m/sec
375.000	0.01000	0.00033	0.00015	299.046	1.58608	2.04800	9.52964	3228.005	2929.914	621.400
375.000	0.00035	0.00155	0.00155	298.235	1.58945	2.05495	8.46516	3226.443	2927.759	620.951
375.000	1.00000	0.003395	0.001612	289.996	1.62439	2.12805	7.38423	3210.541	2915.973	616.370
375.000	10.00000	0.00763	0.025471	193.978	2.13161	3.43629	6.09816	3014.740	2769.418	559.201
375.000	20.00000	0.04020	0.13375	50.977	3.37089	12.97913	5.22456	2600.962	2447.611	443.036
375.000	22.32920	0.32009	0.268390	402	6.17375	1140.34081	4.42460	2096.696	2026.922	272.487
375.000	30.00000	0.558254	0.614226	136.776	3.03118	8.76783	3.53035	1791.439	1737.700	628.391
375.000	40.00000	0.609556	0.751154	262.569	2.92898	6.67753	3.82793	1742.153	1676.531	773.697
375.000	50.00000	0.641323	0.845596	371.204	2.98606	5.92110	3.76322	1716.143	1639.179	872.752
375.000	60.00000	0.665164	0.920369	472.193	2.86293	5.50209	3.71391	1699.482	1609.276	950.597
375.000	70.00000	0.684567	0.983196	562.359	2.84926	5.22670	3.67338	1678.019	1595.765	1015.674
375.000	80.00000	0.701090	1.037796	649.394	2.84092	5.02790	3.63960	1679.908	1565.800	1072.056
375.000	90.00000	0.715576	1.086300	722.320	2.83589	4.87557	3.60794	1674.151	1548.378	1122.066
375.000	100.00000	0.728535	1.130258	811.435	2.83305	4.75396	3.58039	1670.146	1532.884	1167.172
375.000	200.00000	0.816920	1.428529	1490.843	2.84678	4.17620	3.39116	1676.307	1431.485	1478.669
375.000	300.00000	0.873641	1.609018	2051.027	2.87736	3.94928	3.27052	1716.251	1372.860	1677.826
375.000	400.00000	0.917244	1.735453	2544.669	2.90860	3.82040	3.17953	1768.875	1332.756	1828.218
375.000	500.00000	0.953366	1.829497	2993.314	2.93853	3.73586	3.10593	1827.979	1303.538	1950.772
375.000	600.00000	0.984657	1.921525	3408.714	2.96697	3.67609	3.04369	1890.877	1281.527	2055.094
375.000	700.00000	1.012420	1.957411	3798.243	2.99404	3.63191	2.96995	1956.169	1264.756	2146.497
375.000	800.00000	1.037537	2.000840	4166.933	3.01990	3.59836	2.94261	2025.039	1251.962	2228.253
375.000	900.00000	1.060570	2.034292	4518.434	3.04469	3.57244	2.90037	2090.975	1242.374	2302.531
375.000	1000.00000	1.081910	2.059520	4855.496	3.06850	3.55222	2.86230	2159.638	1235.346	2370.847



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